



chain nodes :
 20 21 22 23 24 25 26 27 28 29 31 32 33 35 36 40 41 42 43
 47
 ring nodes :
 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18
 chain bonds :
 1-25 2-40 4-47 10-20 13-23 14-24 15-26 16-22 17-27 18-21 27-28
 27-29 31-32 31-33 31-35 41-42 42-43
 ring bonds :
 1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 8-11 9-10 9-14 11-12
 12-13 12-15 13-14 13-18 15-16 16-17 17-18
 exact/norm bonds :
 1-25 2-40 4-47 5-7 6-10 7-8 8-9 8-11 9-10 9-14 10-20 11-12
 12-13 12-15 13-14 13-18 13-23 14-24 15-16 15-26 16-17 16-22 17-18
 17-27 18-21 27-28 27-29 31-32 31-33 31-35 41-42 42-43
 normalized bonds :
 1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :
 containing 1 :

G1:C,O,S,N

G2:O,S

G3:[*1], [*2]

G4:[*2], [*3]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom
 18:Atom 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS
 26:CLASS 27:CLASS 28:CLASS 29:CLASS 31:CLASS 32:CLASS 33:CLASS
 35:CLASS